Semi-Annual Progress Report

to the

National Aeronautics and Space Administration

in connection with

NASA Grant NGR-47-004-006

to the

Virginia Polytechnic Institute
Blacksburg, Virginia

September 1, 1965

Introduction

Although the Grant was awarded and dated as of March 1, 1965, it was not actually officially received by the Virginia Polytechnic Institute until June 1, 1965. The university advisory group appointed to administer the proposal meet immediately and selected five research proposals for support during the year. These were:

1. Effect of Hydrogen Embrittlement on Static and Dynamic Fatigue of Hollow Specimens (D. H. Pletta, Engineering Mechanics Dept., Principal Investigator)

2. Vibrations of Plates and Shells Composed of Elastic and Viscoelastic Materials. (D. Frederick, Engineering Mechanics Dept., Principal Investigator)

3. Infrared Absorption Due to Impurities and Radiation Damage in Semiconductors (Thomas Gilmer, Physics Dept., Principal Investigator)

4. A Study of Hypersonic Blunt Body Flows (R. T. Davis, Engineering Mechanics Dept., Principal Investigator)

5. Stress Analysis of Shells Under Actual Aerodynamic Loading (F. J. Maher, Engineering Mechanics Dept., Principal investigator)

By the time the grant was officially received, most of the graduate students admitted to graduate school during the summer were committed to other research. Most of the staff whose projects were accepted by the advisory group had made previous plans for the summer. Accordingly, the results at this date are meager, however, some work was done during the summer and all projects will be in full operation with the start of the fall term of school.

Progress reports on three of the projects are attached for review. On the other projects, literature surveys have been started, and in cases where equipment needed to be purchased this has been taken care of for the most part.

APPENDIX A

Infrared Absorption Due to Impurities and Radiation Damage in Semiconductors

Semi-Annual Progress Report

NASA Grant NGR-47-004-006

by

Dr. T. E. Gilmer
Physics Department
Virginia Polytechnic Institute

September 1, 1965

Semi-Annual Progress Report, Project 476 (NASA)

"Infrared Absorption Due to Imputities and Radiation Damage in Semiconductors"

The initial work on this project has consisted of studies in two of the areas given in the proposal:

(1) The lithium-oxygen interaction in silicon has been further investigated, extending the work previously done at this laboratory[1].

(2) The study of the 1s state split in bismuth-doped silicon which was begun before receipt of the contract has been continued.

Equipment has been ordered and most items have been received and installed. In particular, the Perkin-Elmer Model 13 infrared spectrophotometer has been ordered, received and installed. It is now equipped with both sodium chloride and cesium bromide prisms, and thus has a range of 2 to 35 microns. Preliminary absorption spectra have been run on this spectrometer for an initial indication of the oxygen content in silicon samples ordered for future studies.

In the studies of the lithium-oxygen interaction in silicon, two absorption spectra at helium temperatures have been run on samples previously doped and subsequently aged. For one of the samples, SE-3-C, two earlier spectra were available for comparison, and are shown in Figures 1 and 2. These earlier absorptions were run at seven and fourteen days after doping. The new spectrum (Figure 3) in the same region (31-54 microns) corresponds to a sample age of 21 months. A

Figure 1. Absorption Spectrum of Silicon Sample

SE-3-C

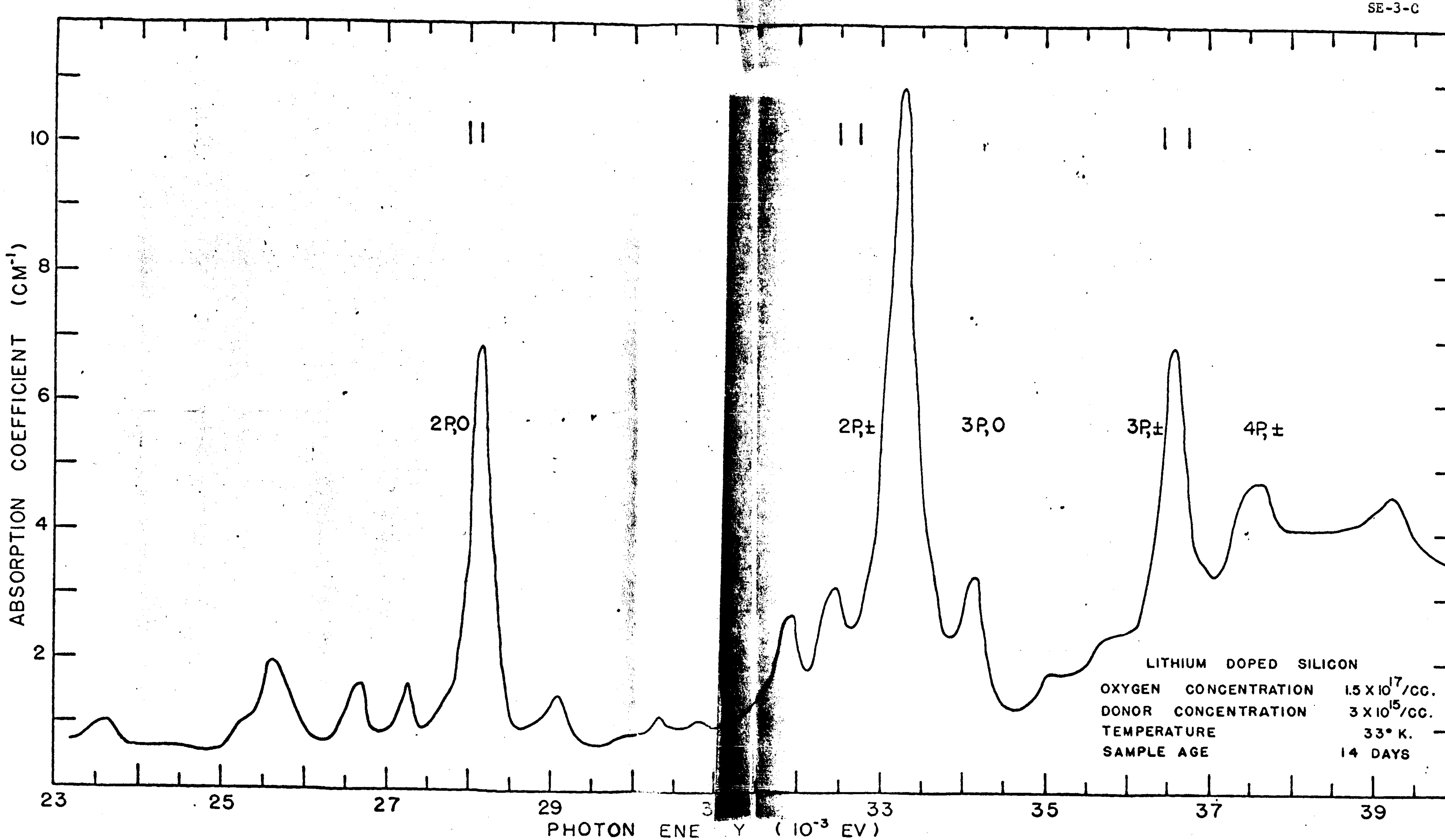


FIGURE 1. ABSORPTION SPECT OF SILICON SAMPLE SE-3-C

Figure 2. Absorption Spectrum of Silicon Sample SE-3-C

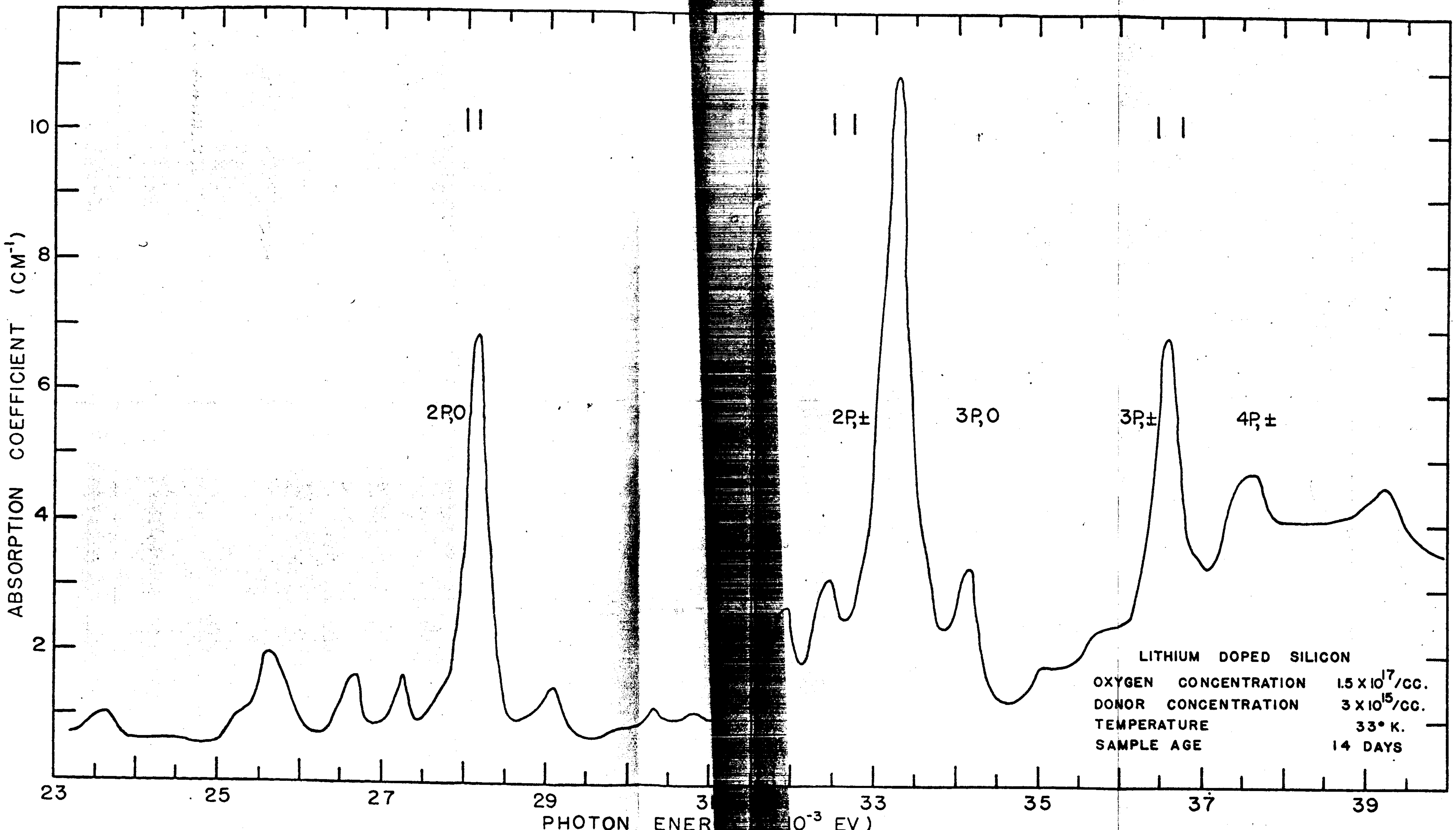


FIGURE 2. ABSORPTION SPECTR[illegible] OF SILICON SAMPLE SE-3-C

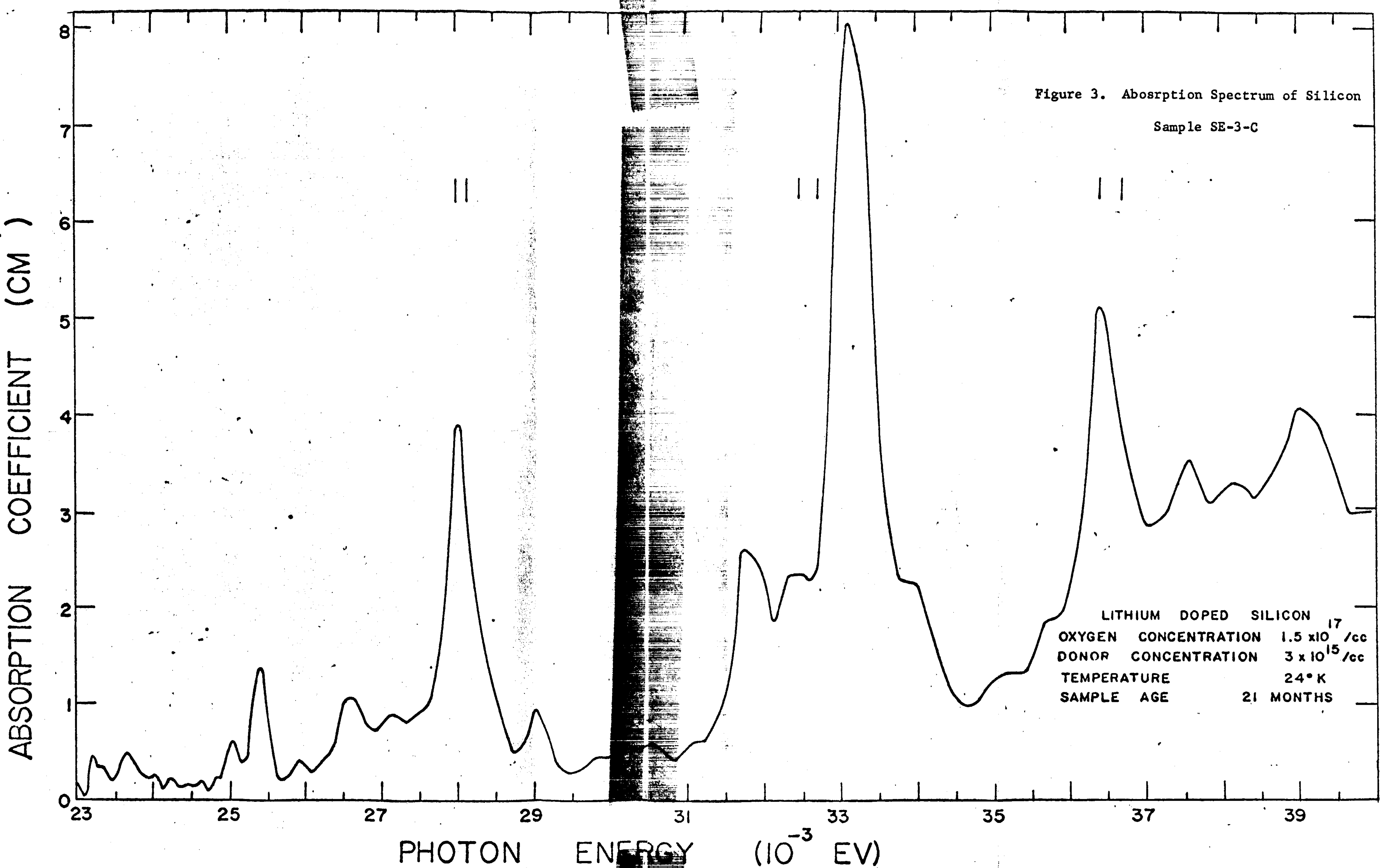


Figure 3. Abosrption Spectrum of Silicon

Sample SE-3-C

ABSORPTION SPECTRUM OF SILICON SAMPLE SE-3-C new spectrum has also been run for a second sample having a higher (3.5×10^{17} cm^{-3}) oxygen concentration than SE-3-C. The data have not yet been reduced; in this case three earlier spectra are available for comparison. Interpretation of the changes in the absorption spectra will not be attempted until more data is available.

In the second area referred to above, that of the studies of bismuth-doped silicon, the preliminary interpretation of the results can be given; more discussion of these studies is thus reported.

The effective mass approximation predicts a six-fold degenerate 1s state, the ground state, for Group V impurities in silicon. Consideration of the site symmetry, T_d, shows that valley-orbit splitting will give rise to singly, doubly and triply degenerate levels, the 1s(A_1), 1s(E) and 1s(T_1) respectively[2]. The 1s(A_1) level is the ground state for Group V impurities. The size of the splitting is dependent on effects in the vicinity of the impurity ion, and the higher 1s(E) and 1s(T_1) levels lie close to the effective mass value of -29×10^{-3} meV for the 1s state energy.

Recent work[3] has given information about the 1s state split in antimony-, arsenic-, and phosphorus-doped silicon. The experiments consisted of observation of the excitation spectra from 1s(E) and 1s(T_1) levels to higher lying states; this requires temperatures high enough to give sufficient population in the 1s(E) and 1s(T_1) states so that observable absorption will occur. For the case of the bismuth impurity in silicon, this approach is more difficult, since the 1s splitting is considerably larger than for the above impurities.

The present experiment gives evidence which may be interpreted as absorption due to transitions from the $1s(A_1)$ level directly to the $1s(T_1)$ level or levels, and perhaps to the 1S(E) level. At the temperatures used, only the $1s(A_1)$ level should have significant population.

The grating spectrometer was purged with dry nitrogen gas both during and for two hours prior to the transmission measurements in order to eliminate water vapor absorptions from the data. In spite of this, some water vapor absorptions are present in our data. The results of this investigation are shown in Figure 4. The data are in the form of absorption spectra in which the absorptions are due only to the impurities introduced into the silicon lattice during the doping process. While bismuth is the desired dopant, we leave open the possibility that other impurities may be present. The spectral slit width is indicated for the regions in which the absorptions occur.

In Figure 4 we note in both curves prominent absorption peaks at 316.5 cm^{-1} and at 273.5 cm^{-1}. The probable explanation of the non-symmetric character of these peaks is that water vapor remained in the system in spite of the fact that the system was purged with the dry nitrogen gas. This is substantiated by the fact that water vapor absorptions do occur at approximately 279 cm^{-1} and 322 cm^{-1}. The rather weak peaks at 342.5 cm^{-1} and 348 cm^{-1} are also in the region of water vapor absorptions.

It is known that phosphorus has absorptions at 316 cm^{-1} and 276 cm^{-1}, leading one to suspect that phosphorus may be present in

Figure 4. Absorption Spectra of Bismuth Doped Silicon

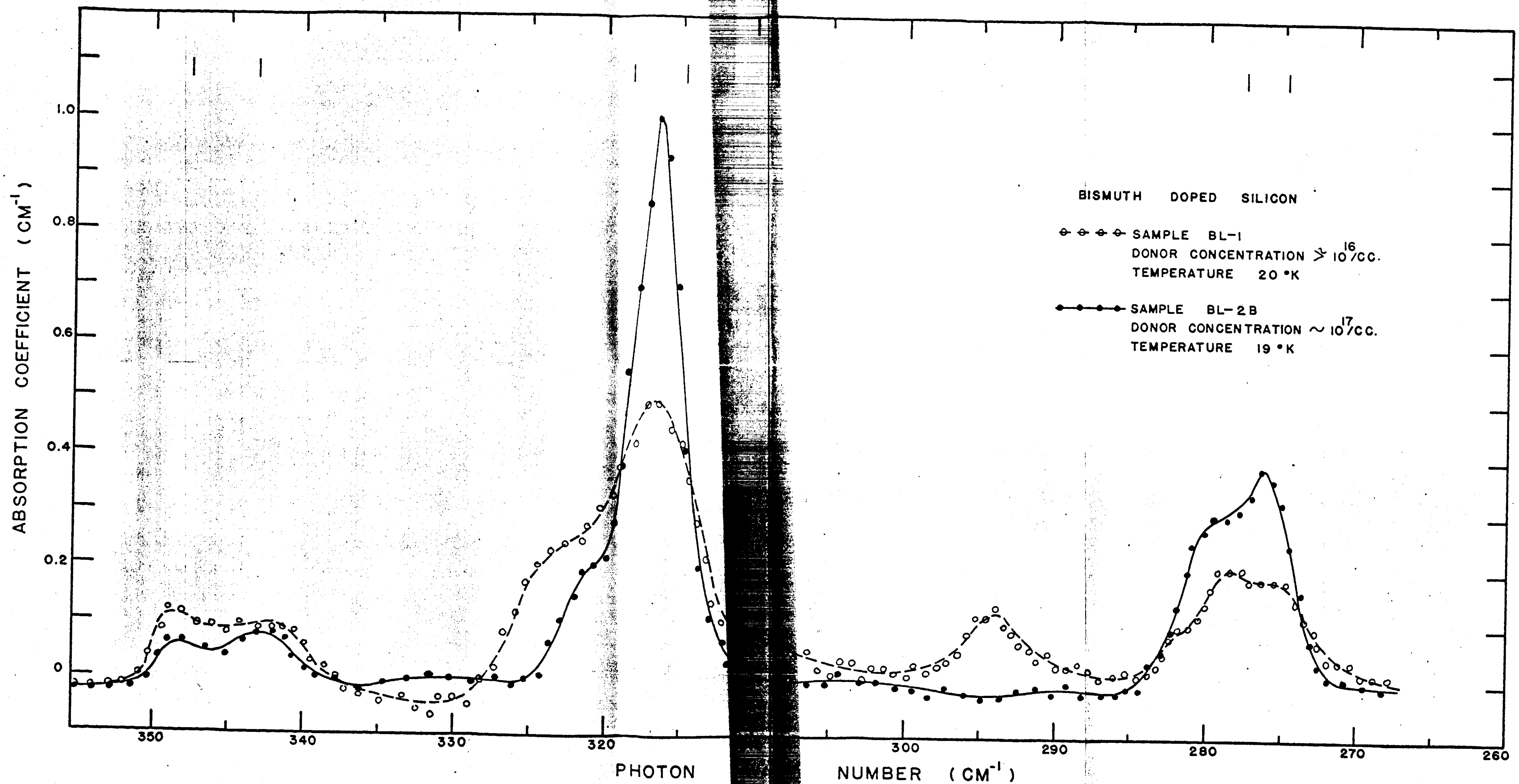


FIGURE 4. ABSORPTION SPE... OF BISMUTH DOPED SILICON

our samples[4]. But phosphorus also has three rather intense absorptions in the range 324 to 350 cm^{-1} and, since these absorptions are not present in our data, we conclude that no significant phosphorus is present in our samples. Antimony has absorptions at 322 cm^{-1} and at 294 cm^{-1} [5]. This leads one to suspect that the large absorption at 316.5 cm^{-1} in our data is due to antimony. However, the antimony absorption at 294 cm^{-1} is almost twice as large as the one at 322 cm^{-1}. We may thus rule out antimony as having any significant effect on our data. It should be noted, however, that a slight amount of antimony in the sample BL-1 would account for the weak absorption at 294 cm^{-1} in the curve for that sample and also for some of the asymmetry of the peak at 316.5 cm^{-1}. Arsenic has no absorptions in the range under consideration and would therefore have no effect on our results[5].

We are thus led to the conclusion that the observed absorptions must be due to the bismuth in the samples. The excited states of bismuth in silicon have been investigated by Hrostowski and Kaiser[6] and by comparing their data with that obtained in this investigation, we conclude that the absorptions in Figure 1 represent transitions from the ground state, $1s(A_1)$, to higher 1s states.

The question in the interpretation is whether the two absorptions are due to $1s(A) \rightarrow 1s(T_1)$ and $1s(A) \rightarrow 1s(E)$ transitions, or whether the $1s(A) \rightarrow 1s(E)$ is in fact strictly forbidden, and the $1s(T_1)$ state is split by a spin-orbit interaction[7]. As shown in Table 1, the observed splitting for bismuth is consistent with other donor splittings also interpreted as 1s(A) to 1s(E) and 1s(T_1) transitions.

Aggarwal[3] has reported observing the 1s state split in antimony-, arsenic-, and phosphorus-doped silicon. His data are listed in Table 1. While we are unable to determine the ordering of the states 1s(E) and 1s(T_1) from our data, we are able to show that the separation of the two states is 5.1×10^{-3} ev, which is of the same order of magnitude as the other values in Table 1. The separation of the ground state, 1s(A_1), from the lowest-lying upper 1s level in our data is 34.1×10^{-3} ev. That this is larger than the other values listed in Table 1 is to be expected because of the large donor ionization energy of bismuth in silicon.

Experiments have also been conducted for the same samples used above in the manner of Aggarwal, i.e. the sample at liquid air temperatures and transitions from the higher 1s states sought. In this case the 1s(E) to higher levels transition would not be forbidden. The experiment, as already indicated, is marginal, and as yet no conclusions have been possible. It is doubtful that any structure in the absorption curve is shown.

Table 1

Energy Spacings of 1s Donor States in Silicon in meV
(Includes values from Ref. 2)

States	Phosphorus	Arsenic	Antimony	Bismuth*
$1s(T_1)$ - $1s(A_1)$	11.85	21.15	9.94	34.1
$1s(E)$ - $1s(T_1)$	1.35	1.42	2.50	5.1

*Assumes $1s(T_1)$ lies below $1s(E)$.

References

1. Gilmer, T. E., Jr., Franks, R. K., and Bell, R. J., "An Optical Study of Lithium and Lithium-Oxygen Complexes as Donor Impurities in Silicon," to appear in J. Phys. Chem. Solids, 1965.

2. Kohn, W., "Shallow Impurity States in Silicon and Germanium," Solid State Physics 5, 257, Academic Press, Inc., New York (1957).

3. Aggarwal, R. L., "Optical Determination of the Valley-Orbit Splitting of the Ground State of Donors in Silicon," Solid State Communications 2, 163, Pergamon Press, Inc., New York (1964).

4. Bichard, J. W. and Giles, J. C., "Optical Absorption Spectra of Arsenic and Phosphorus in Silicon," Canadian Journal of Physics 40, 1481 (1962).

5. Picus, G. S., Burstein, E., and Henvis, B., "Absorption Spectra of Impurities in Silicon -- II, Group V Donors," J. Phys. Chem. Solids 1, 75 (1956).

6. Hrostowski, H. J. and Kaiser, R. H., "Absorption Spectrum of Bismuth-Doped Silicon," J. Phys. Chem. Solids 4, 315 (1958).

7. Krag, W. E. and Zeiger, H. J., "Infrared Absorption of Sulfur-Doped Silicon," Phys. Rev. Lett. 8, 485 (1962).

APPENDIX B

Effect of Hydrogen Embrittlement on Static and Dynamic Fatigue of Hollow Tensile Specimens

Semi-Annual Progress Report

NASA Grant NGR-47-004-006

by

Professor D. H. Pletta
Engineering Mechanics Department
Virginia Polytechnic Institute

September 1, 1965

In Reply Refer To;
SC-NGR-47-004-006

SEMI-ANNUAL REPORT

Effect of Hydrogen Embrittlement on Static and Dynamic Fatigue of Hollow Tensile Specimens

Although this NASA grant was awarded to the V.P.I. Engineering Mechanics Department through the Engineering Experiment Station on March 1, 1965, it was impossible to begin work in a formal way until June because of previous staff assignments. Some preliminary research was done on both the Budd fatigue machine and a Tinius-Olsen Universal testing machine in order to measure the axiality of the longitudinal load vector versus movement of the testing machine head as the load is applied. Even with these precision machines, there is, apparently, a certain amount of load eccentricity which can produce stress variations of $\pm 7\%$ on the extreme fiber at the root of the notch for the specimens contemplated.

These specimens are 0.5 inch diameter notched bars with standard threaded ends as shown in Figure 1. Companion specimens with axial concentric holes of 1/16, 1/8, 3/16, 1/4, and 5/16 inch diameter holes were also used in these preliminary experiments. All of these preliminary tests were made on SAE 1020 steel.

It was possible on the Budd machine to keep the load concentric by adjusting the spherically seated head at one end. All measurements for eccentricity were made by means of SR-4 gauges cemented directly to the test specimens.

Work is now underway to rerun these preliminary tests more precisely and with the use of a special extensometer which is being constructed so that the eccentricity of the load vector may be measured continuously during the test. This work will be rerun on the Olsen and the Budd machines for the static tests and on the Budd machine for the dynamic tests. The character of the fracture surface changed for the notched bars from a flat tensile break for the solid bar to a completely ductile shear lip for the specimen with the 5/16 inch diameter hole. Specimens with smaller sized holes had varying amounts of ductile shear lip fractured surfaces with the remaining being the flat tensile break. The shear lip always occurred at the edge of the inside hole if it did occur at all. Figure 2 shows the variation in the percentage of cross-sectional area with the ductile shear lip fracture plotted versus the geometric scale factor r/R_N where small r = the radius of the hole and capital R_N = the radius of the tensile specimen at the root of the notch.

Quotations are now being obtained for manufacture and heat treatment of the specimens made of SAE 4340 steel. Meanwhile, auxiliary trial specimens are also being fabricated locally in order to reduce the eccentricity factor to as nearly zero as possible.

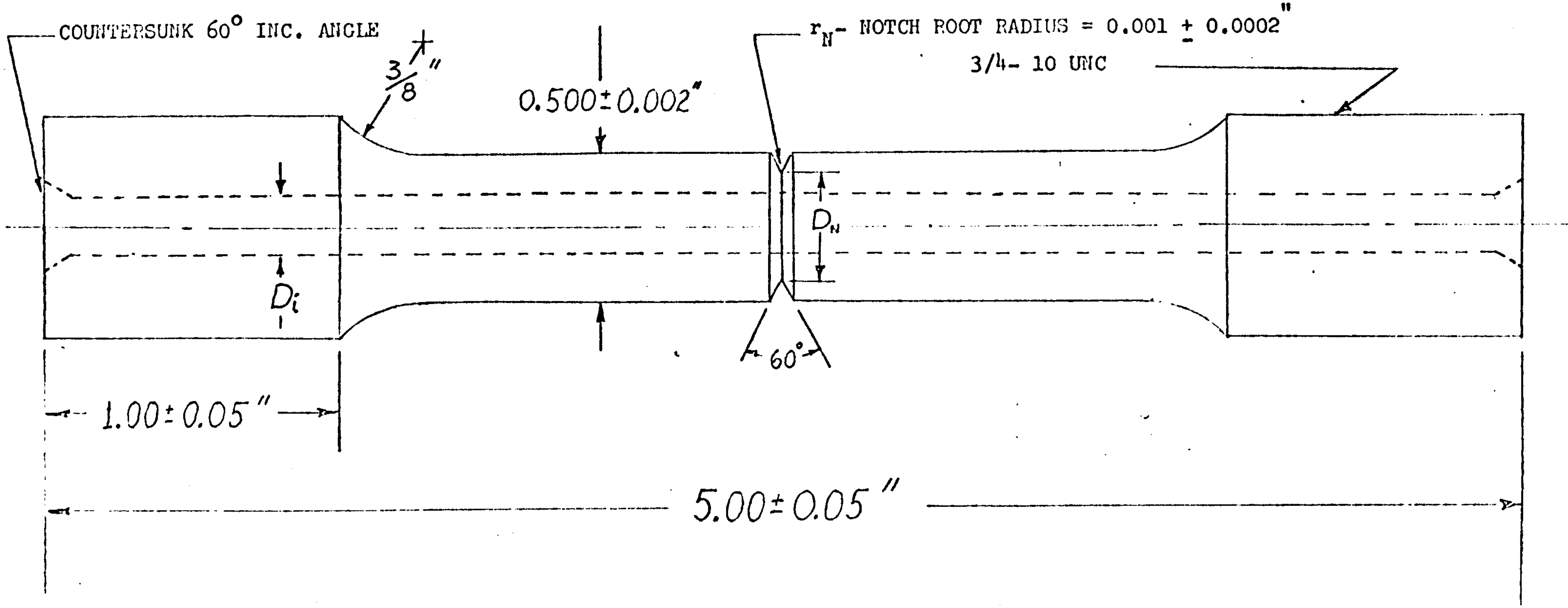
A graduate's assistant has been appointed to work on this project beginning in September.

Respectfully submitted,

R. P. McNitt [signature]
Associate Investigator

D. H. Pletta [signature]
Principal Investigator

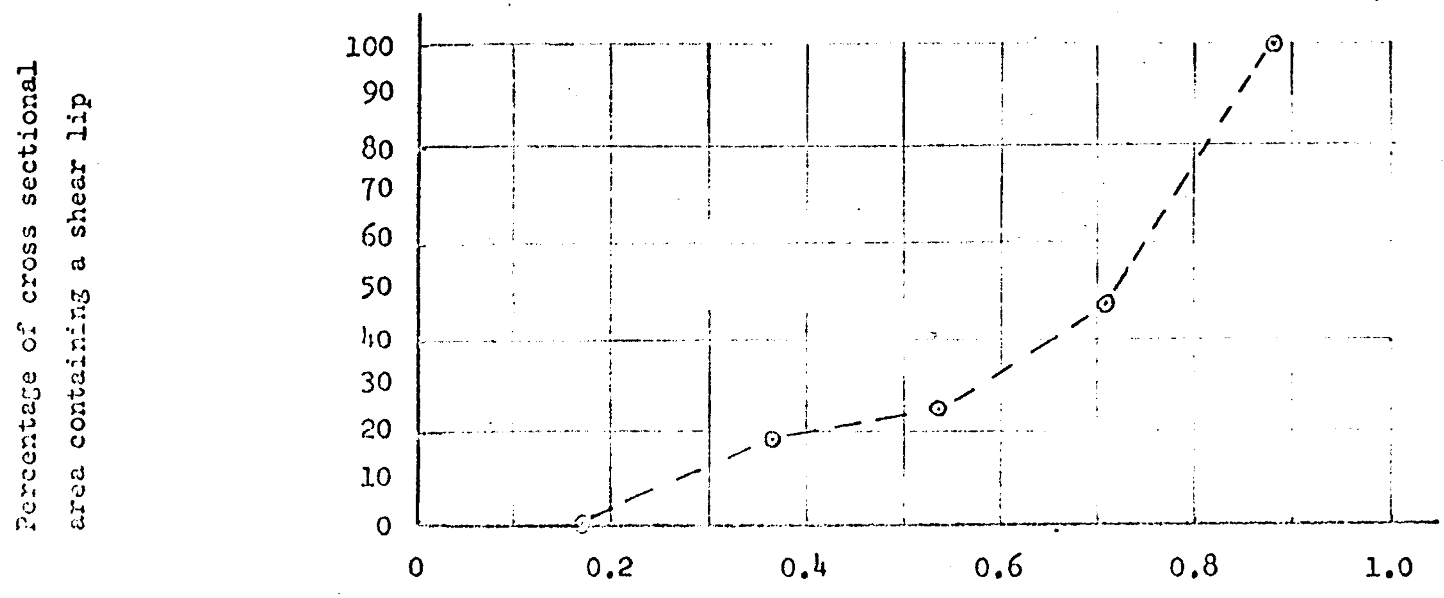
DHP:mmc



D_N = 0.354 ± 0.001"

D_i = 1/16, 1/8, 3/16, 1/4, 5/16 ± 0.001"

FIG 1. TEST SPECIMEN CONFIGURATION



r/R_N

r = Internal hole radius

R_N = Radius of tensile specimen at the root of notch

FIGURE 2 SHEAR FAILURE AREA - FRACTURE AREA RATIO AS A FUNCTION OF NOTCH GEOMETRY

APPENDIX C

A STUDY OF HYPERSONIC BLUNT BODY FLOWS

Semi-Annual Progress Report
NASA Grant NGR-47-004-006

by

Dr. R. T. Davis
Engineering Mechanics Department
Virginia Polytechnic Institute

September 1, 1965

A Study of Hypersonic Blunt Body Flows

The research on this contract was begun on August 1, 1965. Two research assistants were selected and have begun work on the project. A paper titled "Laminar Flow Past a Sphere at High Mock Number" was completed and accepted for publication by the Journal of Fluid Mechanics. An extension of the method used in this paper is being carried out at present for other body shapes and for a compressible fluid. Basically the method consists of simplifying the Navier-Stokes equations so that they are nearly parabolic and then use an implicit finite difference method for the solution of the simplified equations. A copy of the paper is enclosed for those who wish more detail on the method.

The compressible boundary-layer equations have now been programed in fortran in both physical and Levy-Lees variables. These programs are available to NASA upon request.

Another paper co-authored by the principal investigator which was not supported by this grant is enclosed and may be of interest to those interested in approximate boundary-layer methods. This paper has been submitted to ZAMP for publication.